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The hermitian Wilson–Dirac operator in smooth SU(2) instanton backgrounds

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Abstract

We study the spectral flow of the hermitian Wilson–Dirac operator $\mathrm{H}(m)$ as a function of m in smooth SU(2) instanton backgrounds on the lattice. For a single instanton background with Dirichlet boundary conditions on $\mathrm{H}(m)$, we find a level crossing in the spectral flow of $\mathrm{H}(m)$, and we find the shape of the crossing mode at the crossing point to be in good agreement with the zero mode associated with the single instanton background. With anti-periodic boundary conditions on $\mathrm{H}(m)$, we find that the instanton background in the singular gauge has the correct spectral flow but the one in regular gauge does not. We also investigate the spectral flows of two instanton and instanton–anti-instanton backgrounds.

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Key Words: Lattice QCD, Wilson fermions.

1 Introduction

The spectral flow of the hermitian Wilson–Dirac operator $\mathrm{H}(m) = \gamma_5 \mathrm{W}(-m)$ where $\mathrm{W}(m)$ is the conventional Wilson–Dirac operator with bare mass m carries information about the topological content of the background gauge field [1,2] and also carries information about chiral symmetry breaking [3]. Level crossings can occur in the flow for $m > 0$ and the index of the chiral Dirac operator is equal to the net level crossings, in the sense that fermion number is violated by an amount equal to the index. Low lying eigenvalues of $\mathrm{H}(m)$ whether they cross or not can build up a finite density of eigenvalues at zero in the thermodynamic limit and lead to a non-zero chiral condensate. The spectral flow enables one to measure the distribution of the index of the chiral Dirac operator in lattice gauge theories. This has been done for pure SU(2) gauge theory at one value of the lattice coupling [4]. In the continuum,

the index of the chiral Dirac operator is related to the topology of the gauge field background. Assuming this carries over to the lattice, the index of the chiral Dirac operator on the lattice with SU(2) gauge field in the fundamental representation is equal to the topological charge of the gauge field background. The results in [4] provide some support to the above assumption since the distribution of the index obtained there at a fixed gauge coupling is in agreement with the distribution of the topological charge obtained in [5] at the same lattice coupling. In this paper we consider smooth gauge field configurations on the lattice which contain topological objects, with the aim of providing further support to the above assumption. Evidence that SU(2) instantons on the lattice result in level crossings was first observed in Ref. [2]. Low lying eigenvalues of staggered fermion operator have also been used to extract the topological content of background gauge field configurations [6–8]. Low lying eigenvalues of $\mathrm{H}(m)$ in smooth single instanton backgrounds have also been investigated in Ref. [9] with no reference to level crossing.

In this paper we present a systematic study of smooth instanton backgrounds. We study the spectral flow of $\mathrm{H}(m)$ and focus on level crossings to obtain information about the topological charge of the background gauge field. Since we study smooth instanton backgrounds with one or two instantons, we see isolated level crossings and no concentration of eigenvalues near zero. This is not the case in a gauge field background generated from a path integral measure on the lattice [3]. We study the effect of changing the size and the location of the instanton; namely, we consider instantons centered on a lattice site and in the middle of a hypercubic cell. We study the effect of the boundary condition of $\mathrm{H}(m)$ on the spectral flow, and the effect of the gauge choice of the instanton background. In instanton liquid models [10] one builds up a background containing instantons and anti-instantons by summing up gauge field configurations of an appropriate number of instantons and anti-instantons with each in the singular gauge. We study the spectral flow of two instantons and an instanton–anti-instanton background for several separations of the two objects.

2 The hermitian Wilson-Dirac operator

The hermitian Wilson-Dirac operator $\mathrm{H}(m)$ in the chiral basis is

$$\mathrm{H}(m) = \begin{pmatrix} \mathrm{B}-m & \mathrm{C} \\ \mathrm{C}^\dagger & -\mathrm{B}+m \end{pmatrix}; \tag{1}$$

where

$$\mathrm{C}_{i\alpha,j\beta}(n,n') = \frac{1}{2}\sum_\mu \sigma_\mu^{\alpha\beta}[U_\mu^{ij}(n)\delta_{n',n+\hat{\mu}} - (U_\mu^\dagger)^{ij}(n')\delta_{n,n'+\hat{\mu}}] \tag{2}$$

$$\mathrm{B}_{i\alpha,j\beta}(n,n') = \frac{1}{2}\delta_{\alpha,\beta}\sum_\mu [2\delta_{ij}\delta_{nn'} - U_\mu^{ij}(n)\delta_{n',n+\hat{\mu}} - (U_\mu^\dagger)^{ij}(n')\delta_{n,n'+\hat{\mu}}] \tag{3}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};\quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix};\quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};\quad \sigma_4 = \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix}, \tag{4}$$

and where n and n' label the lattice sites, α and β are two component spinor indices, and i and j are three component color indices. We are interested in the eigenvalue problem

$$\mathrm{H}(m)\phi_k(m) = \lambda_k(m)\phi_k(m) \tag{5}$$

as a function of m on a finite lattice. In particular we are interested in level crossings in the spectral flow of $\mathrm{H}(m)$, namely points in m where $\lambda_k(m) = 0$ for some k. All level crossings have to occur in the region $0 \le m \le 8$. Furthermore, any level crossing in the region $0 \le m \le 4$ has an opposite level crossing in the region $4 \le m \le 8$. This is due to the following two facts.

- $\mathrm{H}(m)$ cannot have any zero eigenvalues for $m < 0$.
- The spectrum of $\mathrm{H}(m)$ and $-\mathrm{H}(8-m)$ are the same for an arbitrary gauge field background.

The first one follows from the positive definiteness of B [1]. To see the second one, we note that

$$-\mathrm{H}(8-m,U) = \mathrm{H}(m,-U) = \mathrm{G}^\dagger \mathrm{H}(m,U)\mathrm{G} \tag{6}$$

where

$$\mathrm{G}_{ia,jb}(n,n') = \delta_{ab}\delta_{n,n'}g^{ij}(n); \qquad g^{ij}(n) = \begin{cases} \delta_{ij} & \text{if } \sum_\mu n_\mu \text{ is odd} \\ -\delta_{ij} & \text{if } \sum_\mu n_\mu \text{ is even} \end{cases} \tag{7}$$

is a unitary matrix. Eqn. (6) implies that the spectrum of $-\mathrm{H}(8-m)$ and $\mathrm{H}(m)$ are identical for an arbitrary gauge field background.

3 Instanton backgrounds on the lattice

We will consider gauge field backgrounds that contain instantons. The SU(2) link elements on the lattice obtained from an exact evaluation of the path

ordered integral of the continuum instanton take the following form [8]. In the regular gauge,

$$U_\mu^{\rm reg}(n) = \exp\Big[ia_\mu(n)\cdot\sigma\vartheta_\mu(n;\rho)\Big] \tag{8}$$

$$\vartheta_\mu(n;\rho) = \frac{1}{\sqrt{\rho^2+\sum_{\nu\neq\mu}(n_\nu-c_\nu)^2}}\tan^{-1}\frac{\sqrt{\rho^2+\sum_{\nu\neq\mu}(n_\nu-c_\nu)^2}}{\rho^2+\sum_\nu(n_\nu-c_\nu)^2+(n_\nu-c_\nu)} \tag{9}$$

$$\begin{aligned}
a_1(n) &= (n_4-c_4, n_3-c_3, -n_2+c_2),\\
a_2(n) &= (-n_3+c_3, n_4-c_4, n_1-c_1),\\
a_3(n) &= (n_2-c_2, -n_1+c_1, n_4-c_4),\\
a_4(n) &= (-n_1+c_1, -n_2+c_2, -n_3+c_3)
\end{aligned} \tag{10}$$

and in the singular gauge,

$$U_\mu^{\rm sing}(n) = \exp\Big[ib_\mu(n)\cdot\sigma(\vartheta_\mu(n;0)-\vartheta_\mu(n;\rho))\Big] \tag{11}$$

$$\begin{aligned}
b_1(n) &= (-n_4+c_4, n_3-c_3, -n_2+c_2),\\
b_2(n) &= (-n_3+c_3, -n_4+c_4, n_1-c_1),\\
b_3(n) &= (n_2-c_2, -n_1+c_1, -n_4+c_4),\\
b_4(n) &= (n_1-c_1, n_2-c_2, n_3-c_3)
\end{aligned} \tag{12}$$

$U_\mu^{\rm sing}(n)$ and $U_\mu^{\rm reg}(n)$ are related by the gauge transformation $g(n) = (n_4 + i\sigma_i n_i)/|n|$. Here c denotes the center of the instanton, and ρ is the size of the instanton measured in lattice units. In the regular gauge the non-trivial winding is on the sphere at infinity; however, in the singular gauge the non-trivial winding is localized at c. Instantons in regular gauge can have their center anywhere while instantons in singular gauge cannot have their centers on the lattice site. This is due to the singularity present in $\vartheta(n;0)$ at $n=0$. The anti-instanton is obtained by a parity transformation on the instanton background. We will construct two instanton (instanton–anti-instanton) backgrounds by simply multiplying the gauge field background for a single instanton with the gauge field background for another instanton (an anti-instanton) in the spirit of the dilute gas approximation. For this we will start with the single instantons in the singular gauge since the windings are localized at the center in this gauge and are expected to add when we put instantons together. We will study the spectral flow for two different boundary conditions on $\phi_k(m)$, namely, Dirichlet and anti-periodic. Dirichlet boundary conditions are motivated by the fact that the eigenfuctions are expected to vanish far away from the points where the instantons are localized. Anti-periodic boundary conditions will enable us to study the effect of forcing the geometry of a torus on a non-trivial gauge field background. We use anti-periodic boundary conditions as opposed to periodic

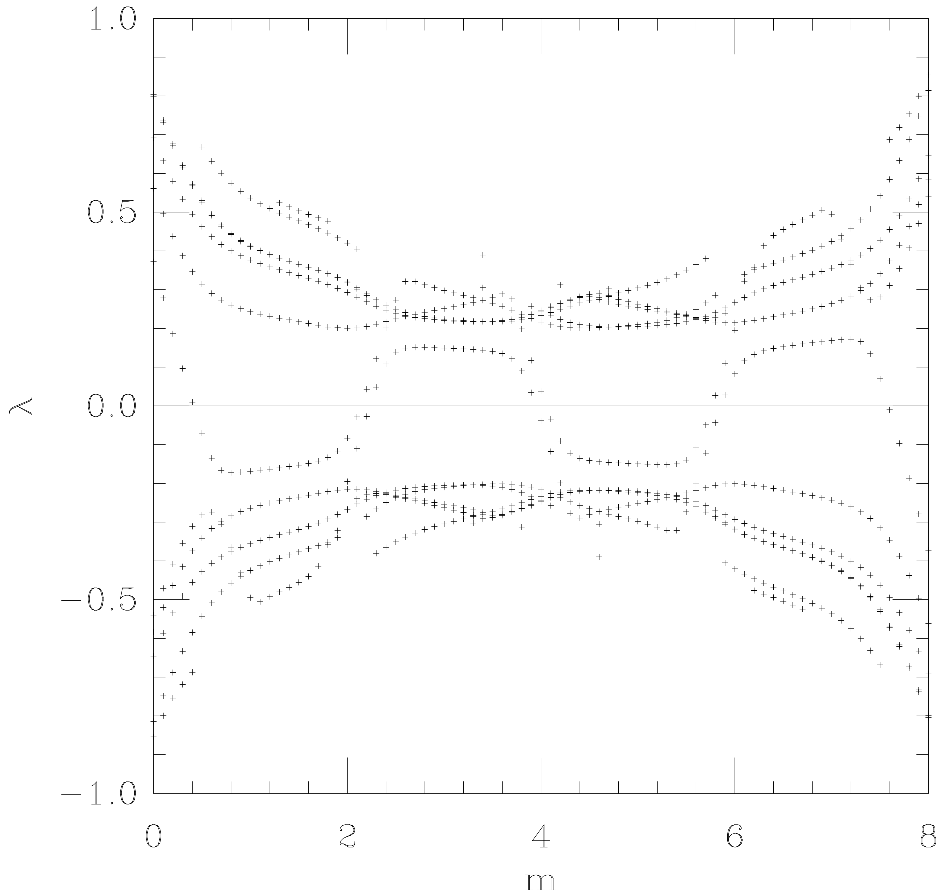

Fig. 1. Spectral flow of H(m) for $0 \leq m \leq 8$ for a single instanton on an 8^4 lattice with Dirichlet boundary conditions for the Wilson fermions. The instanton has a size of $\rho = 2.0$ and is centered at $c_\mu = 4.5$.

boundary conditions to avoid any spurious level crossings from almost zero momentum modes. We use the Lanczos algorithm [11] to obtain the low lying eigenvalues of H(m). We will use the Ritz functional [12] in the neighborhood of level crossings to obtain information about the eigenvectors associated with the levels that cross. The Ritz functional has two advantages over the Lanczos algorithm. The eigenvectors are known in addition to the eigenvalues, and the Ritz functional properly counts any degeneracies in the spectrum.

4 Spectral flow in backgrounds with a single instanton

We start by considering the spectral flow of H(m) in a single instanton background with Dirichlet boundary conditions for H(m). In the continuum the chiral Dirac operator has a single zero mode in this background [13]. If we

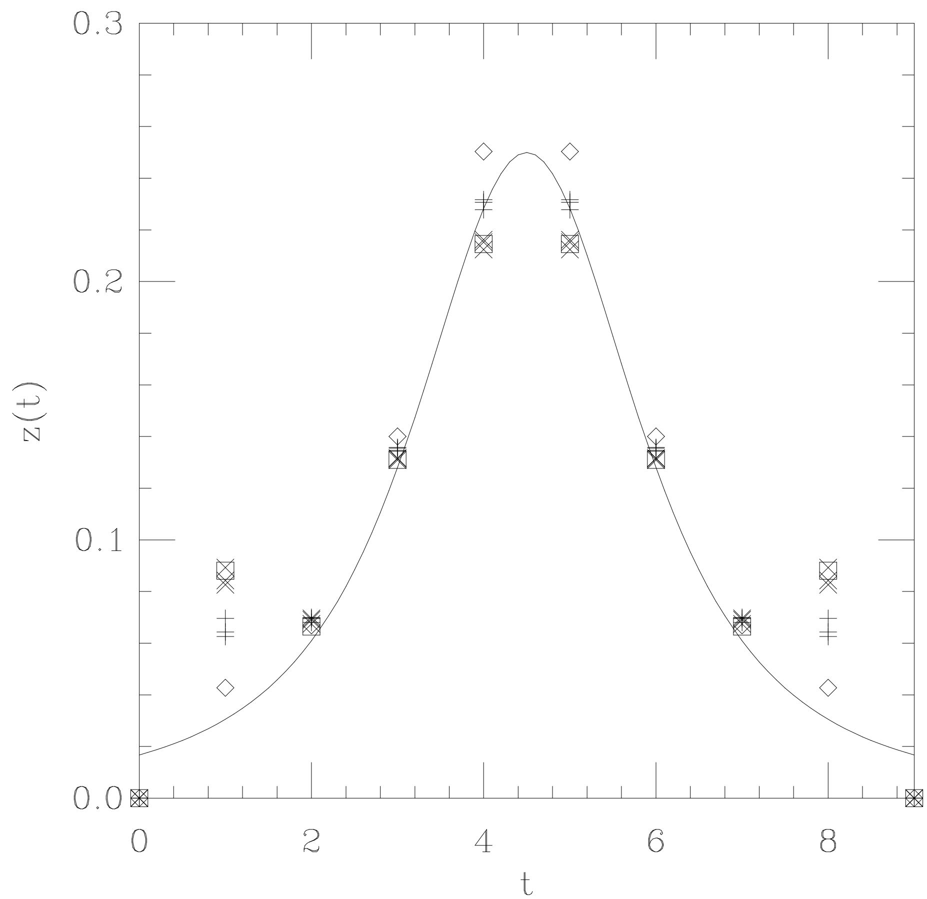

Fig. 2. The modes associated with the level crossings in Fig. 1. The diamond symbol corresponds to the crossing at $m = 0.411$. The square symbol corresponds to the crossing at $m = 2.141$. The three plus symbols correspond to the three degenerate modes crossing at $m = 2.234$. The three cross symbols correspond to the three degenerate modes crossing at $m = 3.949$. The solid line is the zero mode for $\rho = 2.0$ in the continuum.

choose $\rho >> 1$ and consider the spectral flow on a infinite lattice, we expect to find one level crossing close to $m = 0$. Since the free Wilson-Dirac operator effectively describes massless particles also at $m = 2, 4, 6, 8$ we expect four levels to cross near $m = 2$, six levels to cross near $m = 4$ (with three a little before $m = 4$ and three a little after $m = 4$), four levels to cross near $m = 6$ and finally one crossing near $m = 8$. The flow with these crossings will obey the symmetry given by (6). At the crossing points, we have a zero eigenvalue of H(m) and the associate mode should have the appropriate chirality (± 1) and the shape given by the zero mode [13]. From (1) and (5) it follows that

$$\frac{d\lambda_k(m)}{dm} = -\phi_k^\dagger(m)\gamma_5\phi_k(m) \tag{13}$$

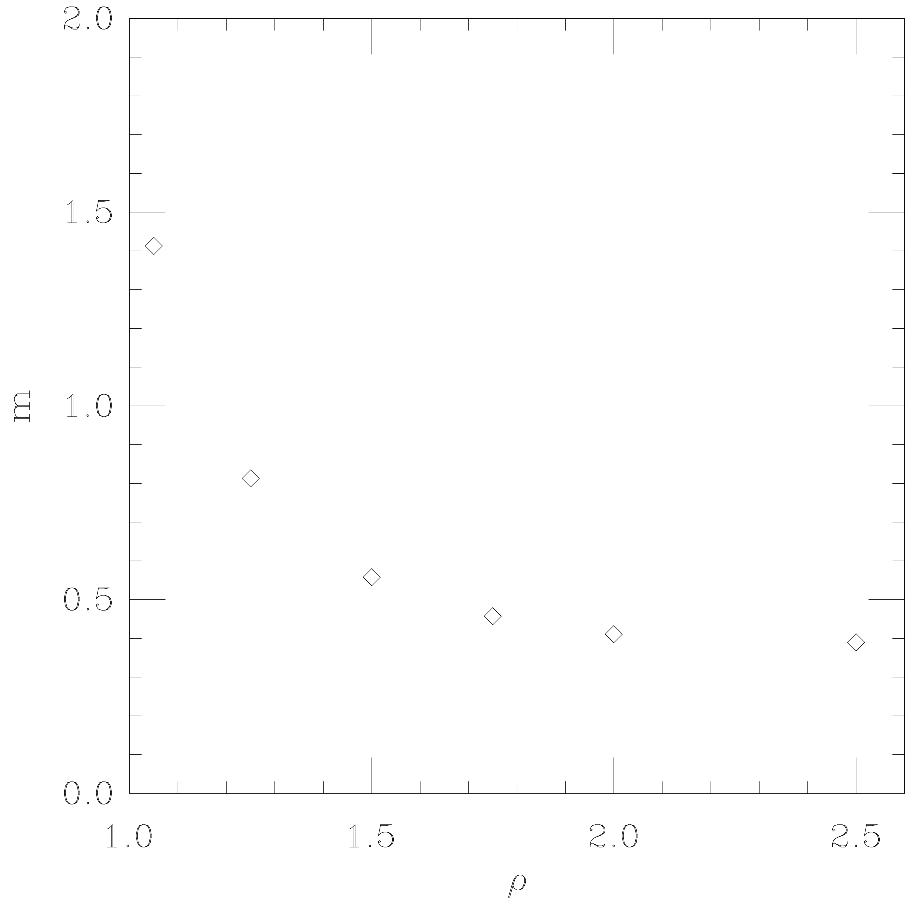

Fig. 3. The crossing point m as a function of ρ for a single instanton centered at $c_\mu = 4.5$ on an 8^4 lattice with Dirichlet boundary conditions imposed on H(m).

and therefore the negative of the slope of the flow at the crossing point gives the chirality of the zero mode.

To verify the above statements, we considered a $\rho = 2$ instanton on an 8^4 lattice with $c_\mu = 4.5$.[1] The flow in the region $0 \le m \le 8$ obtained using the Lanczos algorithm [11] is shown in Fig. 1. We first note that the flow obeys the symmetry given by (6). Using the Ritz functional [12], we studied the modes that cross below $m = 4$. We found that the first downward crossing occurred at $m = 0.411$. This crossing was singly degenerate and the mode had a chirality of 0.829. From there, we found an upward crossing at $m = 2.141$. This crossing was also singly degenerate and the mode had a chirality of -0.707. Next, we found an upward crossing at $m = 2.234$. This crossing was three-fold degenerate and all the modes had chiralities of -0.773. Finally, we found a downward crossing at $m = 3.949$. This crossing was also three-fold degenerate

[1] We label the sites of the lattice from 1 to 8. Therefore, the instanton is positioned in the center of the lattice.

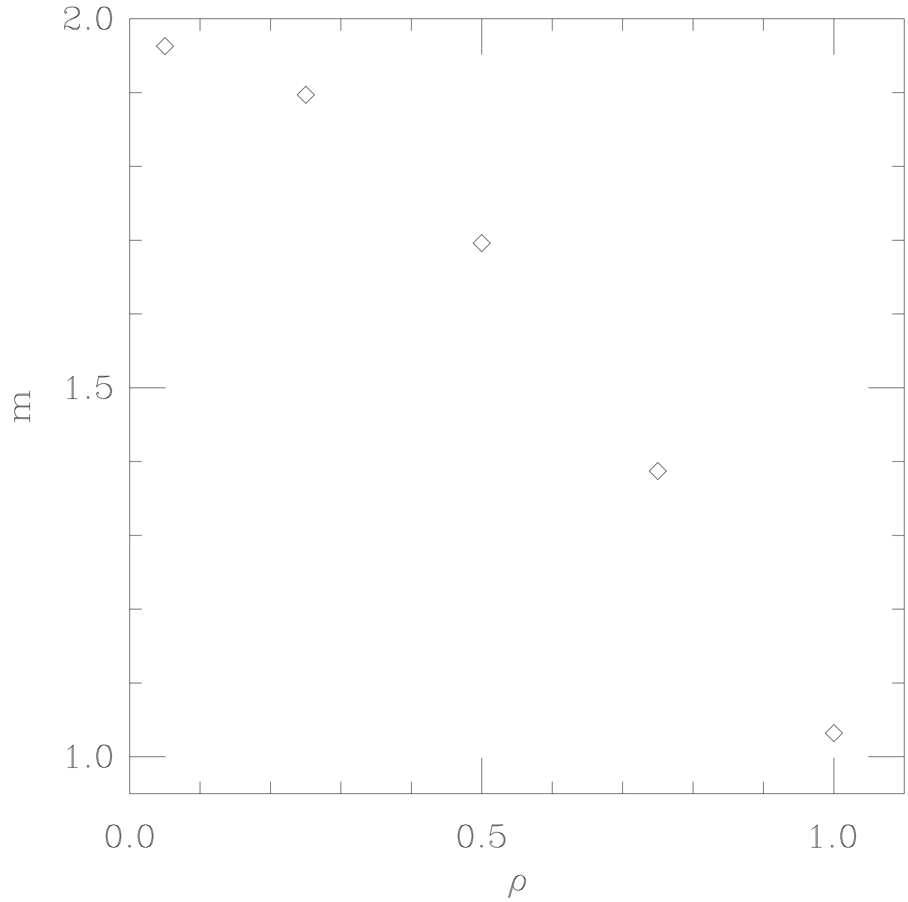

Fig. 4. The crossing point m as a function of ρ for a single instanton centered at $c_\mu = 5$ on an 8^4 lattice with Dirichlet boundary conditions imposed on H(m).

and all the modes had chiralities of 0.715. To verify that these modes are indeed close to the continuum zero modes, we plot $z(t) = \sum_{\vec{n}} \phi_k^\dagger(\vec{n}, t)\phi_k(\vec{n}, t)$ as a function of t in Fig. 2 and compare it with the zero mode in the continuum given by [13]

$$z(t; c, \rho) = \frac{1}{\left[2\rho(1 + (\frac{(t-c_4)}{\rho})^2)^{3/2}\right]} \tag{14}$$

The agreement is excellent. The deviations near the boundary are due to the Dirichlet boundary conditions on the finite lattice imposed at $t = 0$ and $t = 9$.

The agreement between the continuum zero modes and the modes associated with the level crossing is expected to improve as $\rho << L \to \infty$ where L is the linear extent of the lattice. At the crossing point, we obtain the following

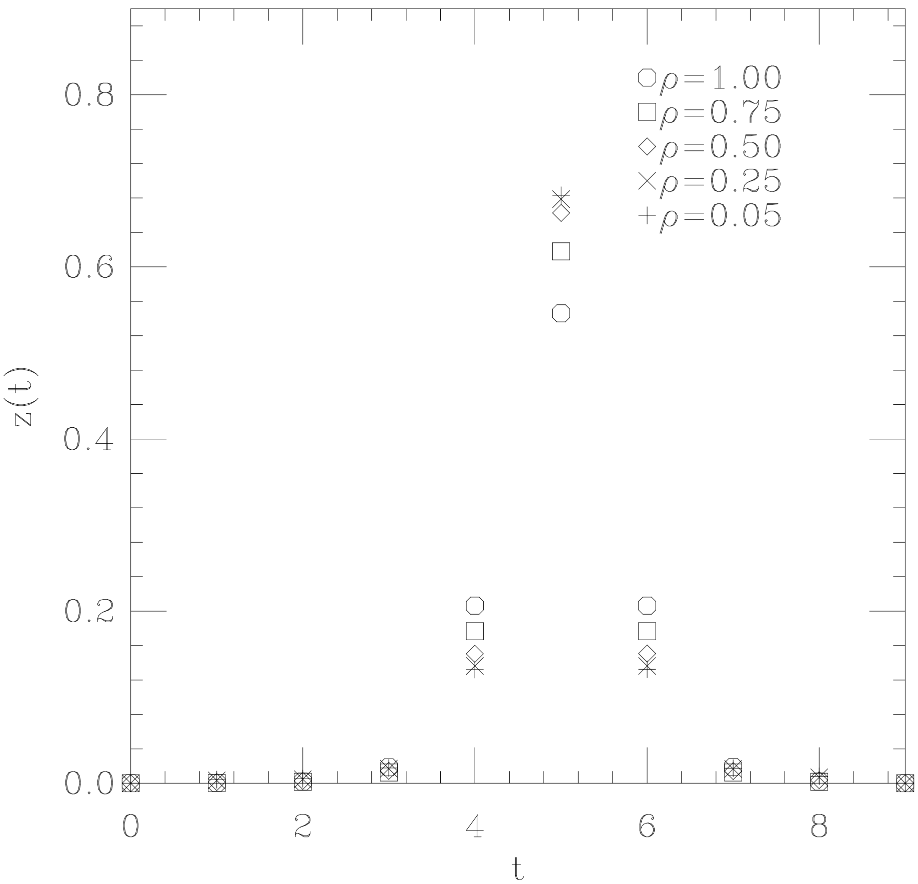

Fig. 5. The modes associated with the points in Fig. 4.

condition from (1) and (5):

$$u^\dagger \mathrm{B} u + v^\dagger \mathrm{B} v = m; \qquad \phi = \begin{pmatrix} u \\ v \end{pmatrix} \tag{15}$$

For larger ρ, ϕ is smoother and we expect the crossing to occur at a smaller m. Fig. 3 provides evidence for this statement. We did not observe any level crossing for $\rho \lesssim 1.0$ instantons implying that instantons centered in the middle of the hypercube "fall through the lattice" if their size is less than about one lattice spacing. As $\rho \to 1$ from above the crossing point in m gets closer to $m = 2$.

To further investigate the fate of instantons smaller than a lattice spacing we considered small instantons centered on a lattice site as opposed to the middle of a hypercube. In Fig. 4 we plot the crossing point as a function of ρ for $\rho \leq 1$ with the instantons centered at $c_\mu = 5$ on an 8^4 lattice. We found a level crossing even for an instanton with $\rho = 0.05$, and the trend in Fig. 4 is consistent with the statement that instantons with smaller ρ result in a

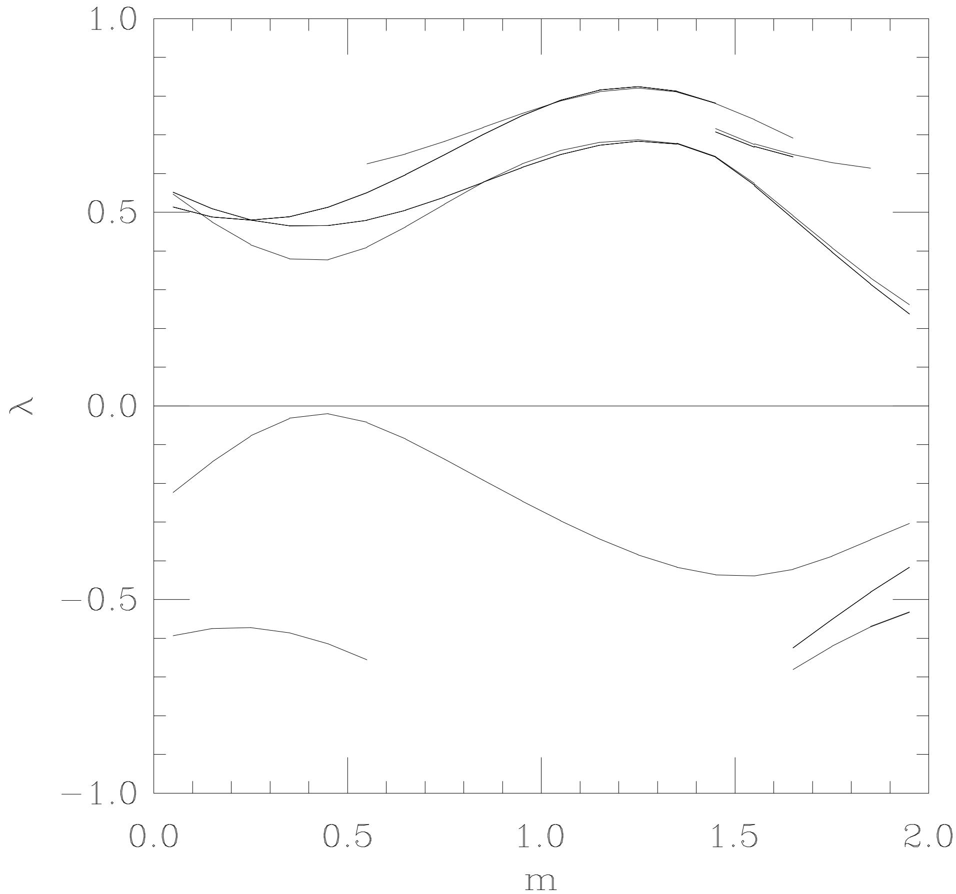

Fig. 6. Spectral flow of H(m) for $0 \leq m \leq 2$ for a single instanton on an 8^4 lattice with anti-periodic boundary conditions for the Wilson fermions. The instanton with a size of $\rho = 1.5$ and centered at $c_\mu = 4.5$ is in the regular gauge.

level crossing at a larger m. However, site centered instantons of a given size cross for a smaller value of m compared to instantons centered in the middle of the hypercube and having the same size. *Instantons do not fall through the lattice if the center of the instanton lies on a lattice site*. However, the mode associated with the level crossing cannot reproduce the continuum mode correctly. From (14) we see that $\frac{z(t=c_4;c,\rho)=1}{2\rho}$ and this diverges as ρ approaches zero. The lattice mode cannot reproduce this singularity. $z(t)$ for the modes associated with the points in Fig. 4 is plotted in Fig. 5. Clearly, the value at $t = 5$ does not grow like $1/\rho$. In fact all these modes roughly look the same and are consistent with a mode of size of about one. The modes at the crossing point for a site centered instanton and a hypercube centered instanton look alike for $\rho > 1$.

The instanton field in the regular gauge and the singular gauge given by (8) and (11), respectively, are proper descriptions on a manifold with a spherical geometry. The gauge potential is equivalent to zero at the origin of the sphere

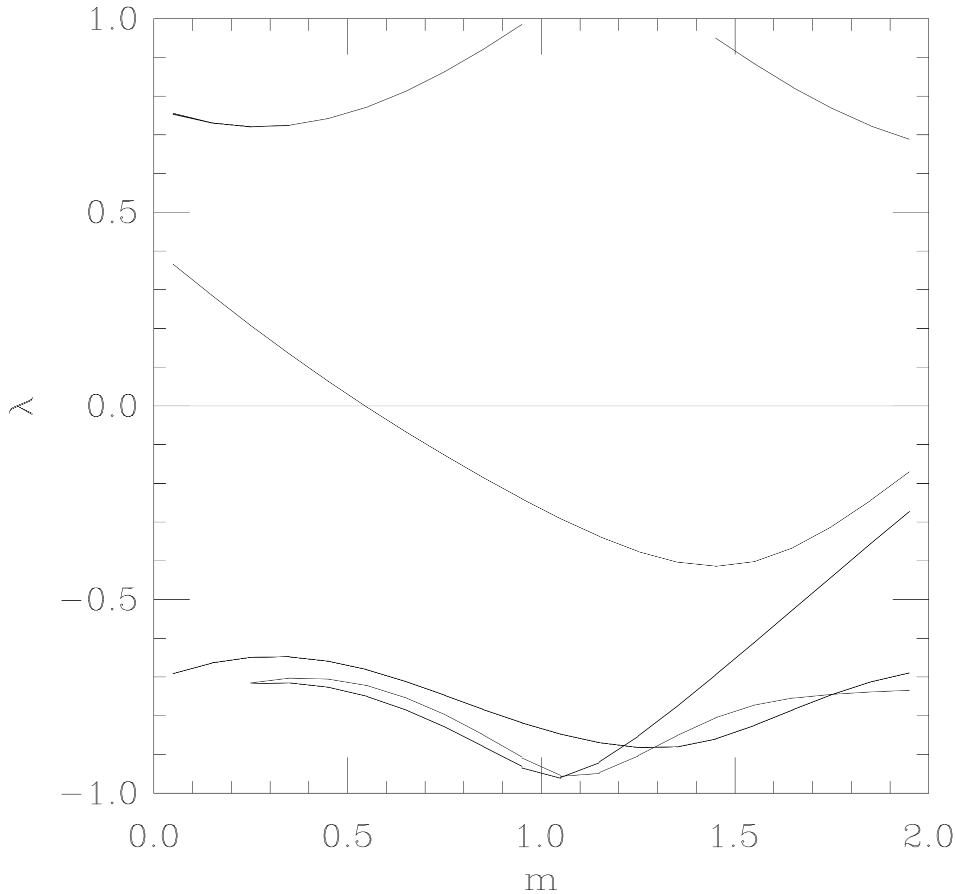

Fig. 7. Spectral flow of H(m) for $0 \leq m \leq 2$ for a single instanton on an 8^4 lattice with anti-periodic boundary conditions for the Wilson fermions. The instanton with a size of $\rho = 1.5$ and centered at $c_\mu = 4.5$ is in the singular gauge.

and on the spherical surface at infinity. The two gauge potentials are related by a non-trivial gauge transformation with a unit winding number. In the regular gauge the winding is at the spherical surface at infinity, and in the singular gauge the winding is localized to the point at the origin of the sphere. In the study of the spectral flow of H(m) with Dirichlet boundary conditions on a finite lattice the gauge choice does not matter. However, the gauge choice is relevant in a study of the spectral flow with anti-periodic boundary conditions. Anti-periodic boundary conditions force a toroidal geometry on a configuration that is well defined only on a spherical geometry. Even if the size of the instanton is much smaller than the lattice size, we expect a radical change in the spectral flow with anti-periodic boundary conditions. Since the action of the gauge field configuration is quite small, periodic boundary conditions cause spurious level crossings due to almost zero momentum modes and this

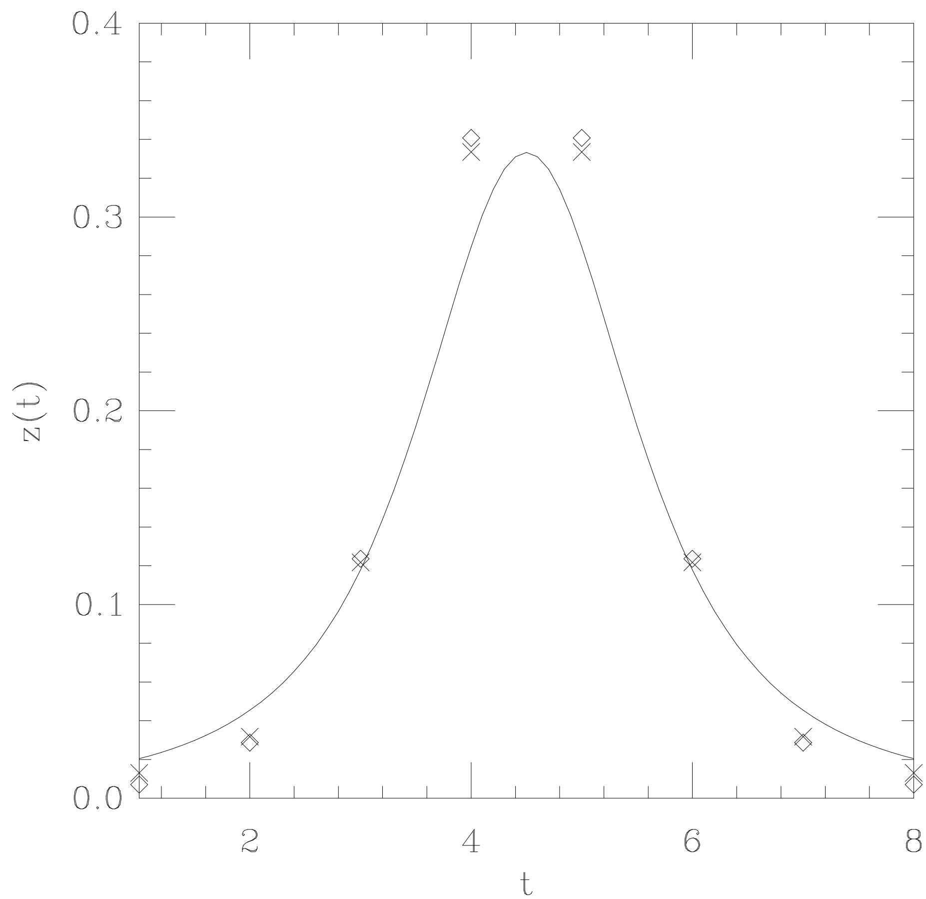

Fig. 8. The mode associated with the level crossing in Fig. 7 is shown with the diamond symbol. The corresponding mode with Dirichlet boundary conditions is shown with the cross symbol and the solid line is the continuum zero mode with $\rho = 1.5$.

is avoided by choosing anti-periodic boundary conditions. [2] The spectral flow for a $\rho = 1.5$ instanton in the regular gauge on an 8^4 lattice with anti-periodic boundary conditions is shown in Fig. 6. The flow for the same instanton in singular gauge is shown in Fig. 7. Fig. 6 shows no crossing indicating that forcing anti-periodic boundary conditions in regular gauge results in loss of the topology. However, Fig. 7 shows one level crossing downward and this is consistent with the topology of a single instanton. The mode associated with this crossing is plotted in Fig. 8. In the same figure we compare this mode with the corresponding mode for the same instanton obtained from the

[2] We studied the spectral flow of $\mathrm{H}(m)$ in a single instanton background with periodic boundary conditions. We found several spurious crossings very close to $m = 0$ and the modes associated with these crossings were very close to a constant mode. Spurious low lying eigenvalues were also observed in the spectrum of the staggered fermion operator with periodic boundary conditions [8].

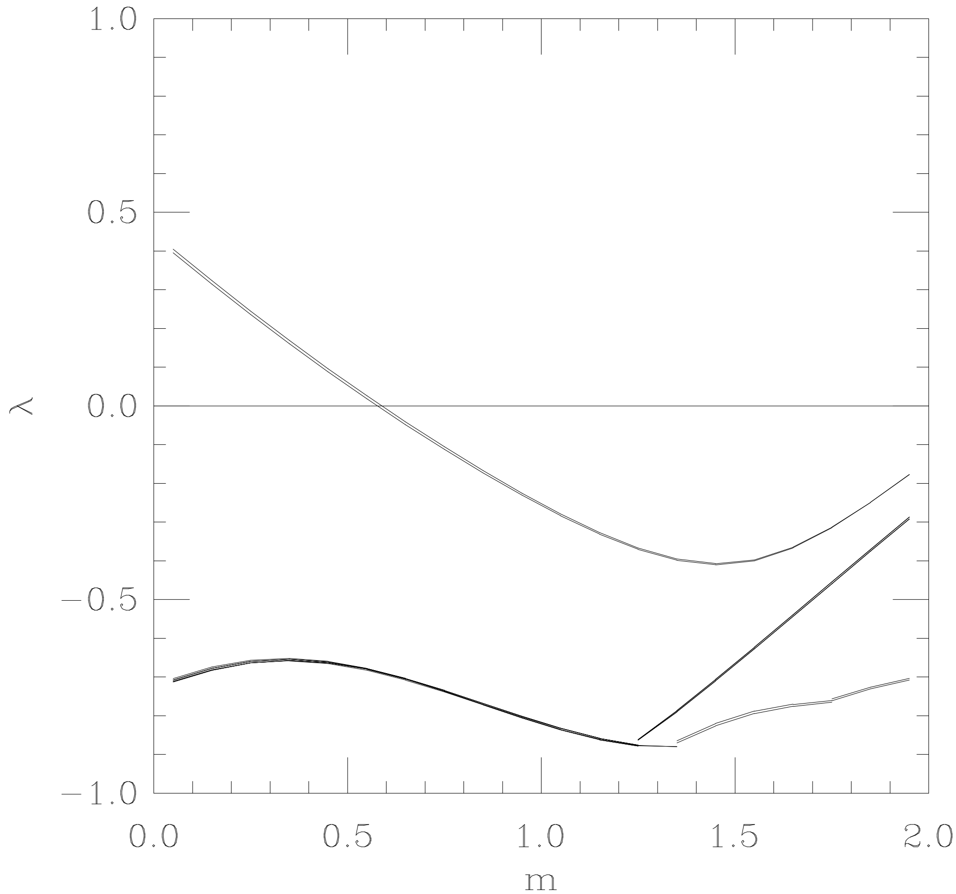

Fig. 9. Spectral flow of H(m) for $0 \leq m \leq 2$ for a two instanton configuration on an 8^4 lattice with anti-periodic boundary conditions for the Wilson fermions. Both instantons have a size of $\rho = 1.5$ and are separated by four lattice spacings in every direction.

spectral flow with Dirichlet boundary conditions. The two modes essentially lie on top of one another and both of them are a proper characterization of the continuum zero mode as shown in Fig. 8. This shows that the topology is not lost by forcing a toroidal geometry if the winding is localized to the point at the center of the instanton. This is consistent with the conclusions obtained from a study of the staggered fermion operator [8]. By studying the spectral flow for various instanton sizes we found that there is no level crossing if the size is less than about one lattice spacing.

5 Spectral flow in backgrounds with two topological objects

In the previous section we established that one can construct a lattice gauge field configuration close to a continuum instanton on a finite lattice with

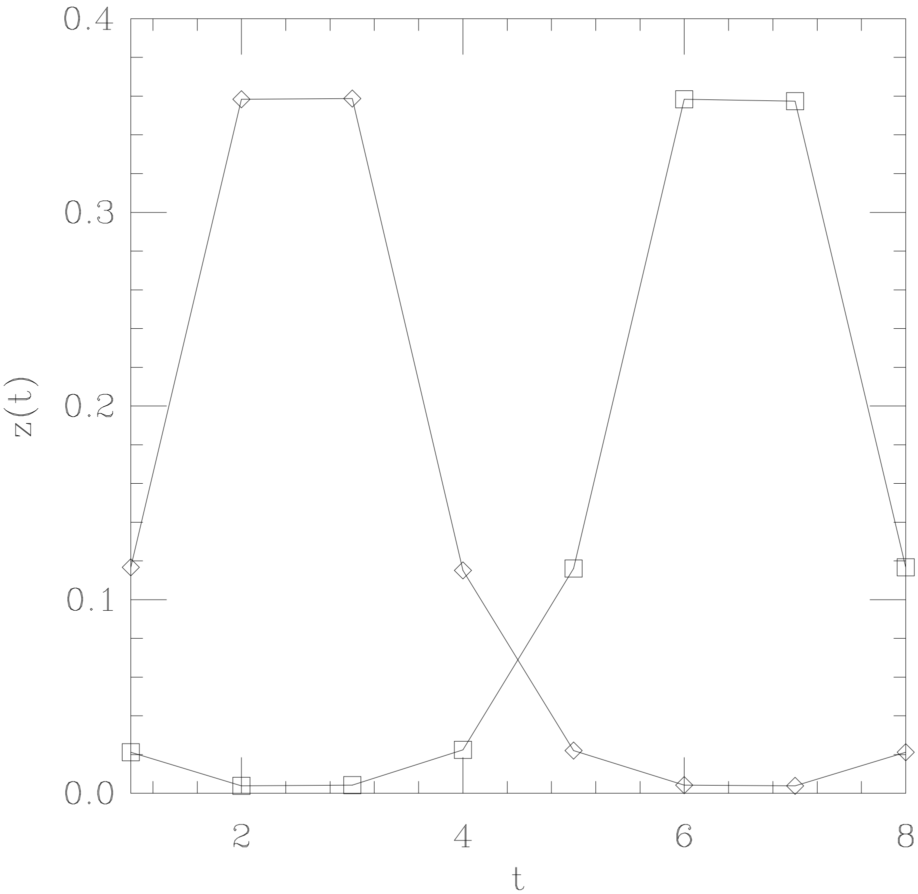

Fig. 10. The modes associated with the level crossings in Fig. 9.

toroidal boundary conditions resulting in a spectral flow of H(m) consistent with the topology. We now turn to two instantons and instanton–anti-instanton configurations as described in section 3. We set both instantons to have the same size, namely $\rho = 1.5$. We consider the spectral flow of H(m) with anti-periodic boundary conditions on an 8^4 lattice. We first consider the situation where the two objects are as far separated as possible on the 8^4 lattice, namely the distance between the two objects is four in all four directions. For the two instanton configuration, we find that two levels cross downward and are almost degenerate. The modes associated with these crossings indeed are very close to the single instanton zero modes with $\rho = 1.5$. The spectral flow is shown in Fig. 9 and the two modes at the crossing point are shown in Fig. 10. For the instanton–anti-instanton configuration we find that one level crosses downwards and another one crosses upwards almost at the same point in m. Like in the two instanton case, these modes are localized at the site of the instanton and anti-instanton and have a size consistent with $\rho = 1.5$. The spectral flow is shown in Fig. 11, and the two modes at the crossing point are shown in Fig. 12. The other extreme is when the two instantons are placed

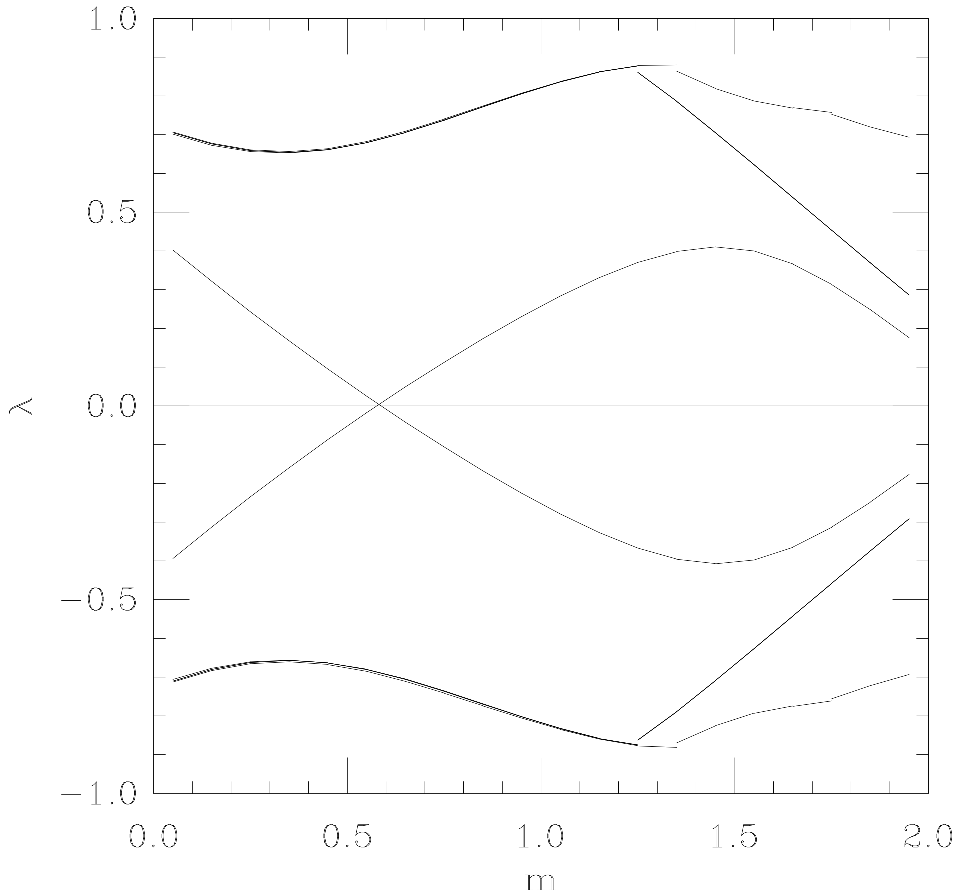

Fig. 11. Spectral flow of H(m) for $0 \leq m \leq 2$ for an instanton–anti-instanton background on an 8^4 lattice with anti-periodic boundary conditions for the Wilson fermions. Both instantons have a size of $\rho = 1.5$ and are separated by four lattice spacings in every direction.

on top of each other. We found only one level crossing downward indicating that the configuration had a topological charge of unity. The mode associated with the crossing is significantly broader than the ones we found for the well separated situations with the size now consistent with $\rho = 1.5 \times \sqrt{2}$. If the two instantons were separated by $(2, 0, 0, 0)$, we still found only one level crossing downward indicating that the configuration still had a topological charge of unity. The mode associated with the crossing was narrower than the case where the instantons were on top of each other, but still broader than the ones found for well separated instantons. When the instantons were separated by $(4, 0, 0, 0)$, we found two crossings indicating that the two instantons were sufficiently separated for them to be resolved as individual instantons. Similar results were found for instanton–anti-instanton configurations. When they were on top of each other no level crossings were observed. When they were separated by a distance of $(2, 0, 0, 0)$ and $(4, 0, 0, 0)$, we found one level crossing downwards and one level crossing upwards indicating that the instanton

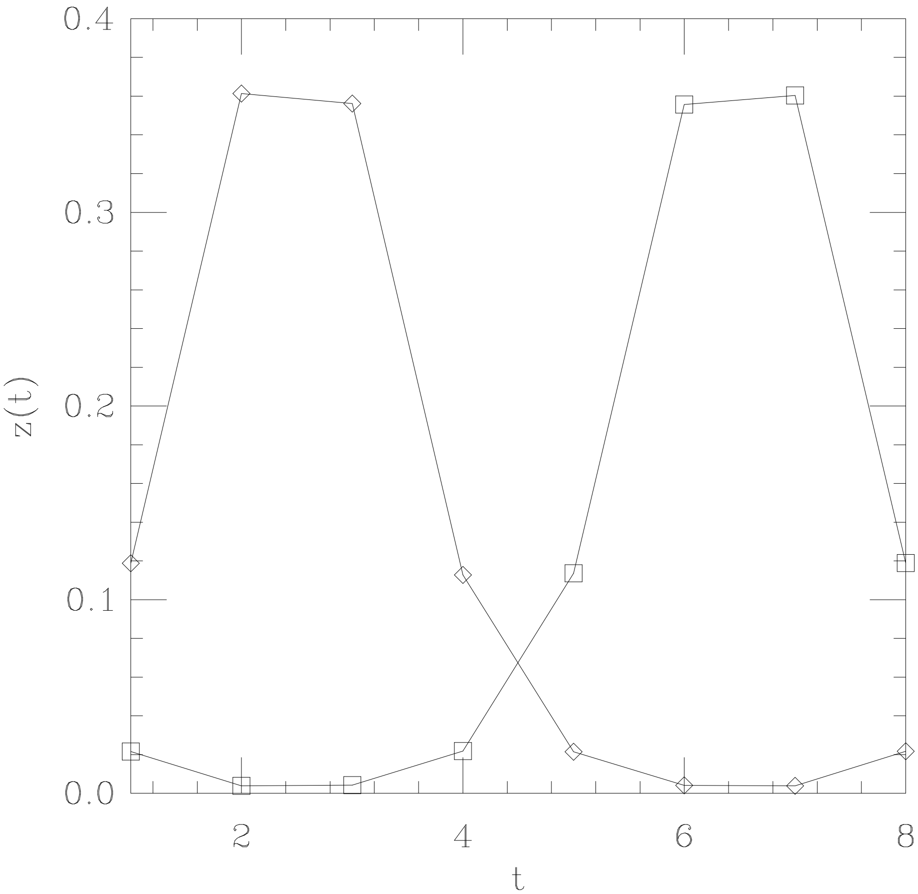

Fig. 12. The modes associated with the level crossings in Fig. 11.

and anti-instanton were resolved for both these separations.

6 Conclusions

We studied the spectral flow of H(m) in smooth instanton backgrounds. For single instanton backgrounds we found the following:

- With Dirichlet boundary conditions for H(m), we found a single level crossing in H(m) with the eigenmode at the crossing point describing a proper realization of the continuum zero mode.
- Instantons with larger sizes resulted in a crossing at smaller values of m, and we found level crossing all the way up to $m = 2$ as we reduced ρ.
- Instantons centered in the middle of a lattice hypercube fell through the lattice if their size was smaller than about one lattice spacing. The Wilson action for these instantons on an open lattice is a monotonic function of ρ with the action going to zero as ρ goes to zero. The action at $\rho = 1$ is well

above the dislocation bound [14] of $12\pi^2/11$.

- Instantons centered on a lattice site never fell through the lattice. This is consistent with the Wilson action for these instantons. It is not a monotonic function of ρ. It has a minimum for a specific value of ρ ($\rho = 1$ on an 8^4 open lattice) below which the action increases. The action never goes below the dislocation bound [14].
- With anti-periodic boundary conditions for H(m), we found that instantons in regular gauge resulted in a gauge field configuration with no level crossing; however, instantons in singular gauge resulted in a single level crossing consistent with the topology.

For two instanton and instanton–anti-instanton backgrounds, we found level crossings consistent with two topological objects if the two instantons were separated by a distance of four or more and if the instanton and anti-instanton were separated by a distance of two or more.

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